

NO-A195 884

MOLECULAR INTERACTIONS WITH MANY-BODY METHODS(U)  
FLORIDA UNIV GAINESVILLE R J BARTLETT 04 MAR 88  
AFOSR-TR-88-0679 AFOSR-85-0011

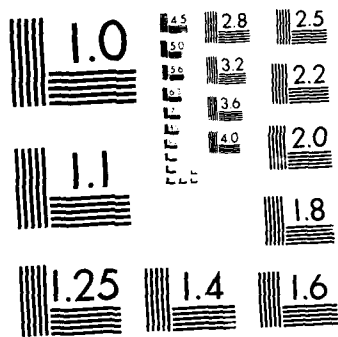
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## REPORT DOCUMENTATION PAGE

AD-A195 684

1b. RESTRICTIVE MARKINGS

3. DISTRIBUTION / AVAILABILITY OF REPORT  
Approved for public release;  
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2b. DECLASSIFICATION / DOWNGRADING SCHEDULE

4. PERFORMING ORGANIZATION REPORT NUMBER(S)

5. MONITORING ORGANIZATION REPORT NUMBER(S)

AFOSR-TR- 88-0679

6a. NAME OF PERFORMING ORGANIZATION

Univ of Florida

6b. OFFICE SYMBOL  
(If applicable)

7a. NAME OF MONITORING ORGANIZATION

AFOSR/NP

6c. ADDRESS (City, State, and ZIP Code)

219 Grinter Hall  
Gainesville, FL 32611

7b. ADDRESS (City, State, and ZIP Code)

Building 410, Bolling AFB DC  
20332-64488a. NAME OF FUNDING / SPONSORING  
ORGANIZATION

AFOSR

8b. OFFICE SYMBOL  
(If applicable)

NP

9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER

AFOSR-85-0011

8c. ADDRESS (City, State, and ZIP Code)

Building 410, Bolling AFB DC  
20332-6448

10. SOURCE OF FUNDING NUMBERS

PROGRAM  
ELEMENT NO.  
61102FPROJECT  
NO.  
2301TASK  
NO.  
A4WORK UNIT  
ACCESSION NO.

11. TITLE (Include Security Classification)

(U) MOLECULAR INTERACTIONS WITH MANY-BODY METHODS

12. PERSONAL AUTHOR(S)

Dr Rodney J. Bartlett

13a. TYPE OF REPORT

FINAL

13b. TIME COVERED

FROM 1 Nov 84 TO 31 Oct 87

14. DATE OF REPORT (Year, Month, Day)

4 Mar 88

15. PAGE COUNT

4

16. SUPPLEMENTARY NOTATION

17. COSATI CODES

FIELD	GROUP	SUB-GROUP
	20.08	

18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

This report summarized publications and invited presentations supported by our AFOSR grant on "Molecular Interactions with Many-Body Methods." In this effort new many-body methods have been developed to treat open-shell molecules; to apply to properties like moments, polarizabilities, hyperpolarizabilities, spin-densities and spin-spin coupling constants; infra-red spectra; and a variety of applications to interesting molecules including the unknown metastable  $N_3H_3$  system. The latter molecule, though isoelectronic with ozone and cyclopropane is not known experimentally. However, we find that it should exist in three stable structures. Furthermore, we have predicted its IR spectra to aid in its experimental identification, which should be possible in matrix isolation. Other applications work has focused on the accurate, numerical orbital treatment of anions. (mjm)

20. DISTRIBUTION / AVAILABILITY OF ABSTRACT

X ☐ UNCLASSIFIED/UNLIMITED ☒ SAME AS RPT ☐ DTIC USERS

21. ABSTRACT SECURITY CLASSIFICATION

UNCLASSIFIED

22a. NAME OF RESPONSIBLE INDIVIDUAL

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22c. OFFICE SYMBOL

AFOSR/NP

DD FORM 1473, 84 MAR

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SECURITY CLASSIFICATION OF THIS PAGE

UNCLASSIFIED

88 6 29 113

## I. PUBLICATIONS AND PRESENTATIONS SUPPORTED BY AFOSR (1986-present)

L. Adamowicz and R.J. Bartlett, "Very Accurate Coupled Cluster Calculations for Diatomic Systems with Numerical Orbitals," Nobel Laureate Symposium on Applied Quantum Chemistry, ed. V.H. Smith, H.F. Schaefer III, and K. Morokumo, Reidel, Dordrecht, The Netherlands, pg. 111 (1986).

S. Kucharski and R.J. Bartlett, "Fifth-Order Many-Body Perturbation and Its Relationship to Various Coupled Cluster Approaches," in Advances in Quantum Chemistry, 18, 281 (1986).

G.W. Trucks and R.J. Bartlett, "Isomers of  $\text{Si}_2\text{C}_2$ : An MBPT Study," Mulliken Issue, J. Mol. Structure (Theochem) 135, 423 (1986).

H. Sekino and R.J. Bartlett, "Hyperpolarizabilities of the Hydrogen Fluoride Molecule: A Discrepancy Between Theory and Experiment?" J. Chem. Phys. 84, 2726 (1986).

D.H. Magers, R.J. Harrison and R.J. Bartlett, "Isomers and Excitation Energies of  $\text{C}_4$ ," J. Chem. Phys. 84, 3284 (1986).

L. Adamowicz and R.J. Bartlett, "Numerical Coupled Hartree-Fock Study of the Total Electronic and Nuclear Parallel Polarizability and Hyperpolarizabilities for  $\text{FH}$ ,  $\text{H}_2^+$ ,  $\text{HD}^+$ , and  $\text{D}_2^+$  Molecules," J. Chem. Phys. 84, 4988 (1986).

L. Adamowicz and R.J. Bartlett, "Accurate Numerical Orbital MBPT/CC Study of the Electron Affinity of Fluorine and the Dissociation Energy of Hydrogen Fluoride," J. Chem. Phys. 84, 6837 (1986).

H. Sekino and R.J. Bartlett, "Frequency Dependent Non-linear Optical Properties of Molecules," J. Chem. Phys. 85, 976 (1986).

L. Adamowicz and R.J. Bartlett, "Coupled-Cluster Calculations of Electron Affinities of  $\text{LiF}$ ," Chem. Phys. Lett. 129, 159 (1986).

H. Sekino and R.J. Bartlett, "Nuclear Spin-Spin Coupling Constants Evaluated Using Many-Body Methods," J. Chem. Phys. 85, 3945 (1986).

L. Adamowicz and R.J. Bartlett, "Direct Coupled Cluster Calculations of Excited States," Int. J. Quantum Chem. Symp. 19, 217 (1986).

E.A. Salter, L. Adamowicz, and R.J. Bartlett, "Comment on MBPT/CC Nickel Calculations," Chem. Phys. Lett. 130, 152 (1986).

S.J. Cole and R.J. Bartlett, "Comparison of MBPT and Coupled-Cluster Methods with Full CI. II. Polarized Basis Sets," J. Chem. Phys. 86, 873 (1987).

J. Noga, R.J. Bartlett and M. Urban, "Towards a Full CCSDT Model for Electron Correlation II. CCSDT-n Models," Chem. Phys. Lett. 134, 126 (1987).

L. Adamowicz and R.J. Bartlett, "MBPT and Coupled-Cluster Calculation on the Neon Atom with Numerical Orbitals," Int. J. Quantum Chem. 31, 173 (1987).

E.A. Salter, H. Sekino and R.J. Bartlett, "Orbital Relaxation and Property Evaluation by Coupled-Cluster Methods," J. Chem. Phys. 87, 502 (1987).

J. Noga and R.J. Bartlett, "The Full CCSDT Model for Molecular Electronic Structure," J. Chem. Phys. 86, 7041 (1987).

M. Rittby and R.J. Bartlett, "An Open-Shell Restricted Coupled-Cluster Method: Application to Ionization Potentials in N<sub>2</sub>," J. Phys. Chem., in press.

L. Adamowicz and R.J. Bartlett, "Excited State Electron Affinities of NaF, LiCl and NaCl," J. Chem. Phys. 88, 313 (1988).

R.J. Bartlett, S.J. Cole, G. D. Purvis, W.C. Ermler, H.C. Hsieh and I. Shavitt, "The Quartic Force Field of H<sub>2</sub>O Determined by Many-Body Methods II. Effects of Triple Excitations," J. Chem. Phys. 87, 6579 (1987).

D.H. Magers, E.A. Salter, R.J. Bartlett, C. Salter, B.A. Hess and L.J. Schaad, "Do Stable Isomers of N<sub>3</sub>H<sub>3</sub> Exist?," J. Am. Chem. Soc., in press.

T. Pluta, A.J. Sadlej and R.J. Bartlett, "Polarizability of OH<sup>-</sup>," Chem. Phys. Lett. 143, 91 (1988).

G.D. Purvis III, H. Sekino and R.J. Bartlett, "Multiplicity of Many-Body Wavefunctions Using Unrestricted Hartree-Fock Reference Functions," Coll. of Czechoslovak Chem. Comm., in press.

M. Urban and R.J. Bartlett, "MBPT and Coupled-Cluster Investigation of Isomerization Reactions: HCN•HNC, BH<sub>3</sub>CH<sup>-</sup>•BH<sub>3</sub>NC<sup>-</sup> and HCNBH<sub>3</sub>•HNCBH<sub>3</sub>," J. Am. Chem. Soc., submitted.

G.W. Trucks, J. Noga and R.J. Bartlett, "Convergence of Coupled Cluster Singles, Doubles and Triples Method," Chem. Phys. Lett., in press.

#### INVITED PRESENTATIONS (1986 - present)

Sept.	1988	ACS Conference on Analytical Derivatives and Molecular Properties, Los Angeles, CA.
Aug.	1988	Sixth International Congress on Quantum Chemistry, Jerusalem, Israel.
June	1988	Workshop on Quantum Chemistry, Basic Aspects, Actual Trends, Girona, Spain.
Feb.	1988	Workshop and Symposium on Aspects of Many-Body Effects in Molecules and Extended Systems, Calcutta, India.
Sept.	1987	National ACS Meeting, Symposium on Bound and Temporary Anions in Chemical Systems, New Orleans, LA.
July	1987	American Conference on Theoretical Chemistry, Gull Lake, MN.
June	1987	The Ninth Annual West Coast Theoretical Chemistry Conference, Berkeley, CA.
May	1987	Fifth School of Advanced Methods of Quantum Chemistry, "Frontiers of Atomic and Molecular Structure Theory," Bachotek, Poland.
April	1987	National ACS Meeting, Symposium on Applications of New Methods for Correlated <u>Ab Initio</u> Studies of Large Molecules, Denver, CO.

April	1987	National APS Meeting, Division of Atomic Molecular and Optical Physics, Symposium on Many-Body Physics, Crystal City, VA.
March	1987	Parr/Eliel Symposium, Chapel Hill, NC.
June	1986	Canadian Symposium on Theoretical Chemistry, Toronto, Ontario, Canada
April	1986	Workshop on Interface between Electronic Structure and Dynamics, Snowbird, Utah.

### III. Non-refereed Papers - None

### IV. Honors

Rodney J. Bartlett has been promoted from Professor to Graduate Research Professor of Chemistry and Physics. The latter rank, which is the highest offered by the University of Florida, is held by only 2% of the faculty.

Three of Dr. Bartlett's papers (published 1978-1981) and supported by AFOSR have recently been designated as Science Citations Classics. Classics are determined by frequency of citation by other scientists and must be among the most cited papers in their respective journals. His paper in *Physica Scripta* 21, 255 (1980), "Molecular Applications of Coupled-Cluster and Many-Body Perturbation Methods," in the Proceedings of Nobel Symposium Issue, is the third most cited paper in the history of that journal, being cited over 160 times. His paper from the *International Journal of Quantum Chemistry* 14, 561 (1978), "Many-Body Perturbation Theory, Coupled Pair Many Electron Theory, and the Importance of Quadruple Excitations for the Correlation Problem," has been cited over 200 times, and is the eighth most cited paper in that journal's history. His review in *Annual reviews of Physical Chemistry* 32, 359 (1981), "Studies of Electron Correlation in Molecules with Many-Body Perturbation Theory and Coupled Cluster Methods," has also been cited over 200 times, and is the twelfth most cited paper in that review series.

### V. Patent Requests - None

### VI. Patents Granted - None

### VII. Students Supported by Grant

D. Bernholdt  
D. Magers  
S. Zarrabian  
E.A. Salter  
G. Trucks  
T. Pluta

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Unannounced	<input type="checkbox"/>
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#### VIII. Postdoctoral Associates Supported by Grant

S. Pal  
M. Rittby  
G. Fitzgerald  
L. Adamowicz  
C. Sosa  
J. Watts  
R.E. Brown (visiting research associate)  
S. Kucharski (visiting research associate)

#### IX. Students Under AFOSR Support Graduated

S. Zarrabian - Convergence to the Solution of the Eigenvalue Problem by  
Perturbative Methods (December, 1987)

E.A. Salter - Analytical One-Electron Response Properties, Molecular  
Gradients and Force Constants in Many-Body Methods  
(May, 1988)

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